

Formyl chloride

2565-30-2 | DTXSID30180344

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	1.14	0.85	1.12	0.83	1.23

Model Results

Predicted value: $2.22\text{e-}13$ cm³/molecule*sec

Global applicability domain: Inside

Local applicability domain index: $2.89\text{e-}01$

Confidence level: $5.67\text{e-}01$

Nearest Neighbors from the Training Set

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Formyl chloride

Measured: $3.20\text{e-}13$

Predicted: $2.22\text{e-}13$

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Chlorofluoromethane

Measured: $4.41\text{e-}14$

Predicted: $4.78\text{e-}14$

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Chloroform

Measured: $1.03\text{e-}13$

Predicted: $6.48\text{e-}14$

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Methane, difluoro-

Measured: $1.09\text{e-}14$

Predicted: $1.56\text{e-}14$

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Formyl fluoride

Measured: $4.00\text{e-}15$

Predicted: $5.19\text{e-}15$